

Hamiltonians for Quantum Computing

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ABSTRACT

We argue that the analog nature of quantum computing makes the usual design approach of constructing complicated logical operations from many simple gates inappropriate. Instead, we propose to design multi-spin quantum gates in which the input and output two-state systems (spins) are not necessarily identical. We outline the design criteria for such devices and then review recent results for single-unit Hamiltonians that accomplish the NOT and XOR functions.

Keywords: Quantum computing, Analog computing, Hamiltonians for quantum gates

1. INTRODUCTION

One of the great challenges of the physics of nanoscale systems has been the design of atomic-size devices operating in a quantum-coherent fashion. Dimensions of semiconductor computer components will soon reach¹ about $0.25\text{ }\mu\text{m} = 2500\text{ }\text{\AA}$, which is well above the atomic sizes at which quantum-mechanical effects are important. However, it is generally expected that as the miniaturization continues, atomic dimensions will be reached. This article concerns with quantum computing, i.e., nanoscale devices that perform logical operations while maintaining quantum coherence. Some early studies^{2,3,4,8,9} considered how quantum mechanics affects the foundations of computer science; issues such as limitations on classical computation due to quantum fluctuations, etc., have been raised. A more recent development^{4,5,6,7,8,9,10,11,12,13,14,15,16,17,18,19,20,21,22,23,24,25,26,27,28,29,30,31,32} has been to utilize the quantum nature of components of atomic dimensions for more efficient computations involving quantum-coherent evolution.

Quantum computing has attracted a lot of interest recently owing to several new features. Firstly, it may be faster than classical computing: new fast quantum algorithms have been proposed.^{33,34,35,36,37} Error correction techniques,^{10,27,33,38,39,40,41,42} unitary operations corresponding to the simplest logic gates,^{5,6,7,8,9,10,11,12,13,14,15,16,17,18,19,20,21,22,23,24,25} and some Hamiltonians for gate operation^{10,11,14,24,28,29,30,31,32,43} have been explored. Ideas on how to combine the simplest quantum gates have been put forth.^{7,15,44} Experimentally, there are several atomic-scale systems where the simplest quantum-gate functions have been recently realized^{26,45,46} or contemplated.¹⁹

There remain, however, many conceptual difficulties with quantum computing.^{4,18} The reversibility of coherent quantum evolution implies that the time scale Δt of the operation of quantum logic gates must be built into the Hamiltonian. As a result, all the proposals available to date assume that computation will be externally timed, i.e., interactions will be switched *on* and *off*, for instance, by laser radiation.

This means that if logical operations are constructed from one or few simple universal gates, then each such gate will have to be precisely controlled from outside. In ordinary classical (i.e., macroscopic, irreversible) computing, the NAND gate is an example of a universal gate. From it complicated logical operations can be constructed. In the classical case, however, it is the internal relaxation processes in the basic gate(s) that determine the time scale of their operation (equilibration) Δt . We consider it extremely unlikely that one would ever be able to control externally, in a coordinated fashion, millions of simple reversible quantum gates in order to operate a macroscopic computer.

Furthermore, quantum computers are naturally *analog*²² in their operation. Indeed, in order to use the power of quantum interference (superposition of states), one has to allow any linear combination of the basis qubit states $|1\rangle$ and $|0\rangle$. Analog errors are difficult to correct. By analog errors we mean those minor variations in the input and output variables which cannot on their own be identified as erroneous in an analog device because its operation involves *continuous* values of variables (so that the fluctuated values are as legal as the original ones). By noise errors we term those that result from single-event problems with device operation, or from external influences (including

decoherence in the quantum case), or from other failures in operation. All errors in a *digital* device (i.e., deviations from discrete values) can be systematically decreased or eliminated in each step of a calculation. Similarly, the noise errors in analog devices can be corrected or decreased.

However, the analog errors cannot be corrected. Consider a state $\alpha|1\rangle + \beta|0\rangle$ and a nearby state $\alpha'|1\rangle + \beta'|0\rangle + \sum_j \zeta_j |j\rangle$, where α' is close to α , β' is close to β , while ζ_j are small. The latter terms represent admixture of quantum states $|j\rangle$ other than the two qubit states. Both states are equally legal as input and output quantum states. We could restrict input or output to a vicinity of certain states, for instance, the basis states $|1\rangle$ and $|0\rangle$, thus moving towards digitalization. However, we then lose the quantum-interference property. Another important effect: decoherence, that would require a density matrix description, falls in the noise-error category.

Modern error-correction techniques^{10,27,33,38,39,40,41,42} can handle the noise errors but not the analog errors. To illustrate, consider this quote⁴² from the article entitled *Quantum Error Correction for Communication*: “To achieve this the sender can add two qubits, initially both in state $|0\rangle$, to the original qubit and then perform an encoding unitary transformation...”. The problem here is that the states actually encountered in the system during error correction are not available as basis qubit states (such as $|0\rangle$) with infinite precision. Typically, by qubits we mean a set of two orthogonal quantum states selected from the energy eigenstates of the system. Even assuming that the thermal noise can be reduced at low temperatures to make the ground state sufficiently long-lived, the excited states of any system, especially if it is a part of a macroscopic computer, will not be defined sharply enough to provide ideal stationary states $|1\rangle$ and $|0\rangle$. External interactions, spontaneous emissions, etc., will generate both noise- and analog-errors in the basis states, i.e., the actual state (disregarding decoherence) will be $\alpha|1\rangle + \beta|0\rangle + \sum_j \zeta_j |j\rangle$, with $\alpha \simeq 1$ and $\beta, \zeta_j \simeq 0$, instead of the ideal $|1\rangle$ which is an eigenstate of an ideal, isolated-system Hamiltonian.

Furthermore, analog errors will be magnified when separate simple-gate operations are combined to yield a complex logical function. Thus, the conventional picture of a quantum computer is unrealistic: it assumes a multitude of simple-gate units each being externally controlled by laser beams (one needs a lot of graduate students for that!). Such computers will magnify analog errors which cannot be corrected in principle because the error state is as legal as the original state.

In this work we therefore adopt a view typical of the analog-computer approach, of designing the computer as a single unit performing in one shot a complex logical task instead of a chain of simple gate tasks. This approach will not repair all the ailments outlined earlier. For instance, the computer as a whole will still be subject to analog errors. However, these will not be magnified by proliferation of sub-steps each of which must be exactly controlled.

In fact, we consider it likely that technological advances might first allow design and manufacturing of limited-size units, based on several tens of atomic two-level systems, operating in a quantum-coherent fashion over a sufficiently large time interval to function as parts of a larger classical (dissipative) computer which will not maintain a quantum-coherent operation over its macroscopic dimensions. We would like these to function as single analog units rather than being composed of many gates.

The outline of this review is as follows. In Section 2 we continue our discussion of the design of quantum gates. In Section 3 we review known results for the simplest NOT gate mainly to set the notation and nomenclature. A more complicated, two-spin NOT gate is studied in Section 4. Section 5 addresses the time-dependence of the Hamiltonians. Finally, Sections 6, 7, 8 review results for a three-spin XOR gate.

2. DESIGN CONSIDERATIONS FOR MULTI-SPIN QUANTUM GATES

In order to make connections with the classical computer-circuitry design and identify, at least initially, which multi-qubit systems are of interest, we propose to consider spatially extended multi-spin quantum gates with input and output qubits possibly different. The reason for emphasizing this property is that multi-spin devices will have spatial extent. The interactions that feed the input need not be identical to those interactions/measurements that read off the output. Furthermore, for systems with short-range interactions one can only access the boundary spins in a large cluster. Thus we may use only part of the spins to specify the input and another subset to contain the output. The two sets may be identical, partially overlapping, or nonoverlapping.

Reversibility of coherent quantum evolution makes the distinction between the input and output less important than in irreversible computer components. However, we consider the notion of separate (or at least not necessarily

fully identical) input and output useful within our general goals: to learn what kind of interactions are involved and to consider also units that might be connected to/as in classical (dissipative) computer devices.

Our goal is to be able to design interaction parameters, presumably by numerical simulations, to have such gates perform useful Boolean operations. This is not an easy task. Actually, it must be broken into several steps. First, we must identify those interactions which can be realized in solid state or other experimental arrangements. As examples below illustrate for several simplest gates the form of the interaction Hamiltonians is quite unusual by the solid-state standards.

Secondly, we expect interactions to be short-range and two-particle (two-spin) when several two-state systems (termed qubits, spins) are involved.

Thirdly, incorporating designed coherent computational units in a larger classical computer will require a whole new branch of computer engineering because the built-in Boolean functions will be complicated as compared to the conventional NOT, AND, OR, NAND, etc., to which computer designers are accustomed. Furthermore, the rules of their interconnection with each other and with the rest of the classical computer will be different from today's devices.

Our initial studies have been analytical. In the future we foresee numerical studies of systems of order 20 to 25 two-state (spin) atomic components with variable general-parameter interactions. In this review we summarize results^{28,31,32} for interaction Hamiltonians required for operation of the NOT (Sections 3,4) and XOR (Sections 6, 7, 8) logic gates. Other results presently available include Hamiltonians for certain NOT^{14,28} and controlled-NOT gates,^{10,30,43} and for some copying processes,^{29,30} as well as general analyses of possibility of construction of quantum computing systems.^{8,22}

Quantum logics and the dynamics of quantum gates should be fully reversible. Implications of this property have biased recent literature on the quantum logic gates. Firstly, the distinction between the input and the output parts of the system has been blurred. A typical configuration involves a quantum-mechanical system that is “programmed” with the input and then after the time interval Δt it will be in the output state. We note that the time interval Δt is fully determined by the parameters of the Hamiltonian; in order to effect the quantum gate operation, the interaction energies associated with both the internal and external-field parts of the Hamiltonian must be of order $\hbar/\Delta t$.

Consideration of multi-spin quantum gates requires a large number of basis states. However, it is also useful to study few-spin exactly solvable systems. These provide explicit examples of what the actual interaction Hamiltonians should look like. A notable exactly solvable system, known before the quantum-computing field became active, is the NOT gate operation in a two-state qubit¹⁴ obtained by applying a constant external magnetic field to a single spin. Then another field is applied, oscillating in time, in a direction perpendicular to the constant field. This *paramagnetic resonance* problem is a textbook example of time-dependent quantum-mechanical evolution.

An accepted approach has been to consider interactions switched on only for the duration of the gate operation Δt . If the gate is actually the whole computer then one can regard the interaction as time-independent. However, for specific tasks in components with a limited number of basis states, it may be appropriate to view the interaction as controlled externally to be switched on and off. While general ideas of externally timed computation are not new,⁴ actual realizations in quantum computation with many sub-unit gates will encounter difficulties outlined earlier. General developments for the latter type of interaction (time-independent or on/off) have included^{8,22} identification of unitary operators that correspond to quantum computer operation and establishment of the existence of the appropriate interaction Hamiltonians.

A quantum gate performs an operation whereby the input state determines the output state after a time interval Δt . The interactions must be controlled, i.e., switched on and off, in order to have the gate operation during the interval Δt independent of the interactions with the computer parts external to the gate. This control of interaction, i.e., external timing of the computer operation already mentioned earlier, can be possibly accomplished by the external interactions while the internal interactions be reserved for the gate operation. However, we would like to consider multi-spin gates in order to avoid too many such controlling external influences.

With regards to the requirement to control the interactions externally, with the time dependence given by the on/off protocol, we will show in Section 5 how to extend this approach to certain time-dependent interactions (protocols) which are more smooth than the on/off shape.

3. THE SIMPLEST NOT GATE

In this section we consider the NOT gate²⁸ based on a single qubit. This gate has been extensively studied in the literature.^{5,7,13,14,15,22} Our presentation here is only intended to set up the notation and illustrate methods useful in more complicated situations addressed in Sections 4, 6, 7, 8. We label by $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and $\begin{pmatrix} 0 \\ 1 \end{pmatrix}$ the two basis states. The NOT gate corresponds to those interactions which, over the time interval Δt , accomplish the following:

$$\begin{pmatrix} 1 \\ 0 \end{pmatrix} \Rightarrow e^{i\alpha} \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \quad (1)$$

$$\begin{pmatrix} 0 \\ 1 \end{pmatrix} \Rightarrow e^{i\beta} \begin{pmatrix} 1 \\ 0 \end{pmatrix}. \quad (2)$$

Here α and β are arbitrary. The unitary matrix U that corresponds to this evolution is

$$U = \begin{pmatrix} 0 & e^{i\beta} \\ e^{i\alpha} & 0 \end{pmatrix}, \quad (3)$$

with the eigenvalues

$$u_1 = e^{i(\alpha+\beta)/2} \quad \text{and} \quad u_2 = -e^{i(\alpha+\beta)/2}, \quad (4)$$

while the normalized eigenvectors yield the transformation matrix T which can be used to diagonalize U :

$$T = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{i\beta/2} & e^{i\beta/2} \\ e^{i\alpha/2} & -e^{i\alpha/2} \end{pmatrix}. \quad (5)$$

We have

$$T^\dagger U T = \begin{pmatrix} u_1 & 0 \\ 0 & u_2 \end{pmatrix}. \quad (6)$$

Here the dagger superscript denotes Hermitian conjugation.

We next use the relation

$$U = e^{-iH\Delta t/\hbar} \quad (7)$$

for a time-independent Hamiltonian. In the diagonal representation, it yields the energy levels:

$$E_1 = -\frac{\hbar}{2\Delta t}(\alpha + \beta) + \frac{2\pi\hbar}{\Delta t}N_1, \quad E_2 = -\frac{\hbar}{2\Delta t}(\alpha + \beta) + \frac{2\pi\hbar}{\Delta t}\left(N_2 + \frac{1}{2}\right), \quad (8)$$

where N_1 and N_2 are arbitrary integers. The Hamiltonian is then obtained from the relation

$$H = T \begin{pmatrix} E_1 & 0 \\ 0 & E_2 \end{pmatrix} T^\dagger \quad (9)$$

as a certain 2×2 matrix. The latter is conveniently represented in terms of the unit matrix \mathcal{I} and the conventional Pauli matrices σ_x , σ_y , σ_z :

$$H = \left[-\frac{\hbar}{2\Delta t}(\alpha + \beta) + \frac{\pi\hbar}{\Delta t}\left(N_1 + N_2 + \frac{1}{2}\right) \right] \mathcal{I} + \frac{\pi\hbar}{\Delta t}\left(N_1 - N_2 - \frac{1}{2}\right) \left[\left(\cos \frac{\alpha - \beta}{2} \right) \sigma_x + \left(\sin \frac{\alpha - \beta}{2} \right) \sigma_y \right]. \quad (10)$$

To effect the gate operation, the interaction must be switched on for the time interval Δt . The constant part of the Hamiltonian only affects the average phase $\frac{\alpha+\beta}{2}$ of the transformation (1)-(2). Thus this term can be disregarded.

The nontrivial part of (10) depends on the integer $N = N_1 - N_2$ which is arbitrary, and on one arbitrary variable

$$\gamma = \frac{\alpha - \beta}{2}. \quad (11)$$

Thus we can use the Hamiltonian

$$H = \frac{\pi\hbar}{\Delta t} \left(N - \frac{1}{2} \right) [(\cos \gamma) \sigma_x + (\sin \gamma) \sigma_y]. \quad (12)$$

For a spin- $\frac{1}{2}$ two-state system such an interaction can be obtained by applying a magnetic field oriented in the xy -plane at an angle γ with the x -axis. The strength of the field is inversely proportional to the desired time interval Δt , and various allowed field values are determined by the choice of N .

We note that during application of the external field the *up* and *down* quantum states in (1)-(2) are not the eigenstates of the Hamiltonian. If the time interval Δt is not short enough, the energy-level splitting $|E_1 - E_2| \propto |N - \frac{1}{2}|$ can result in spontaneous emission which is one of the sources of errors in computer operation. Generally, when implemented in condensed matter, the two states of the qubit may be part of a spectrum of many energy levels. In order to minimize the number of spontaneous transition modes, the best choice of the interaction strength would correspond to minimizing $|E_1 - E_2|$, i.e., to $|N - \frac{1}{2}| = \frac{1}{2}$.

4. THE SPATIALLY EXTENDED TWO-SPIN NOT GATE

In this section we consider a more complicated situation. Two two-state systems, input (I) and output (O), are involved. We will use the following self-explanatory notation for the state vector:

$$\begin{aligned} \begin{pmatrix} a_1 \\ a_2 \\ a_3 \\ a_4 \end{pmatrix} &= a_1 |\uparrow\uparrow\rangle + a_2 |\uparrow\downarrow\rangle + a_3 |\downarrow\uparrow\rangle + a_4 |\downarrow\downarrow\rangle \\ &= a_1 \begin{pmatrix} 1 \\ 0 \end{pmatrix}_I \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix}_O + a_2 \begin{pmatrix} 1 \\ 0 \end{pmatrix}_I \otimes \begin{pmatrix} 0 \\ 1 \end{pmatrix}_O + a_3 \begin{pmatrix} 0 \\ 1 \end{pmatrix}_I \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix}_O + a_4 \begin{pmatrix} 0 \\ 1 \end{pmatrix}_I \otimes \begin{pmatrix} 0 \\ 1 \end{pmatrix}_O. \end{aligned} \quad (13)$$

In what follows we will omit the direct-product symbols \otimes when multiplying expressions with subscripts I and O .

We seek transformations such that irrespective of the initial state of O , and provided I is initially in the up or down state, the final state has O in the down or up state, respectively (while the final state of I is not restricted). Thus, we place the logical NOT of I in O provided the initial state of I was one of the basis states corresponding to the classical bit values 1 and 0. The desired transformation maps any state with $a_3 = a_4 = 0$ into a state with components 1 and 3 equal zero, i.e., input up yields output down. Similarly, any state with $a_1 = a_2 = 0$ should evolve into a state with components 2 and 4 equal zero, corresponding to input down giving output up. The general evolution operator must therefore be of the form

$$U = \begin{pmatrix} 0 & 0 & U_{13} & U_{14} \\ U_{21} & U_{22} & 0 & 0 \\ 0 & 0 & U_{33} & U_{34} \\ U_{41} & U_{42} & 0 & 0 \end{pmatrix}, \quad (14)$$

which depends on 16 real parameters. However, one can show that the requirement of unitarity, $U^\dagger U = 1$, imposes 8 conditions so that the number of real parameters is reduced to 8. The following parametrization covers all such unitary matrices:

$$U = \begin{pmatrix} 0 & 0 & e^{i\chi} \sin \Omega & e^{i\beta} \cos \Omega \\ -e^{i(\alpha+\rho-\eta)} \sin \Upsilon & e^{i\rho} \cos \Upsilon & 0 & 0 \\ 0 & 0 & e^{i\delta} \cos \Omega & -e^{i(\beta+\delta-\chi)} \sin \Omega \\ e^{i\alpha} \cos \Upsilon & e^{i\eta} \sin \Upsilon & 0 & 0 \end{pmatrix}. \quad (15)$$

Here all the variables are unrestricted; we could limit Ω and Υ to the range $[0, \frac{\pi}{2}]$ without loss of generality.

In order to make the calculation analytically tractable, we will restrict the number of free parameters to four by considering the matrix

$$U = \begin{pmatrix} 0 & 0 & 0 & e^{i\beta} \\ 0 & e^{i\rho} & 0 & 0 \\ 0 & 0 & e^{i\delta} & 0 \\ e^{i\alpha} & 0 & 0 & 0 \end{pmatrix}. \quad (16)$$

This form has been favored for a possible analytical calculation for the following reasons. Firstly, the structure of a single phase-factor in each column is similar to that of the two-dimensional (single-spin) matrix encountered earlier. Secondly, the form (16) contains Hermitian- U cases ($\beta = -\alpha$, $\rho = 0$ or π , $\delta = 0$ or π). Therefore, the eigenvalues, which are generally on the unit circle for any unitary matrix, may be positioned symmetrically with respect to the real axis, as functions of the parameters. Indeed, the eigenvalues of U turn out to be quite simple:

$$u_1 = e^{i(\alpha+\beta)/2}, \quad u_2 = -e^{i(\alpha+\beta)/2}, \quad u_3 = e^{i\rho}, \quad u_4 = e^{i\delta}. \quad (17)$$

The (unitary) diagonalizing matrix T is

$$T = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{i\beta/2} & e^{i\beta/2} & 0 & 0 \\ 0 & 0 & \sqrt{2} & 0 \\ 0 & 0 & 0 & \sqrt{2} \\ e^{i\alpha/2} & -e^{i\alpha/2} & 0 & 0 \end{pmatrix}. \quad (18)$$

The next step is to identify the energy levels. We chose the notation such that the energies $E_{1,2}$ are identical to (8). The other two energies are given by

$$E_3 = -\frac{\hbar}{\Delta t} \rho + \frac{2\pi\hbar}{\Delta t} N_3, \quad E_4 = -\frac{\hbar}{\Delta t} \delta + \frac{2\pi\hbar}{\Delta t} N_4. \quad (19)$$

The Hamiltonian is then obtained as in the single-spin NOT case. It is convenient to avoid cumbersome expressions by expressing it in terms of the energies; the latter will be replaced by explicit expressions (8), (19) when needed. The resulting 4×4 matrix has been expressed in terms of the direct products involving the unit matrices and the Pauli matrices of the input and output two-state systems. We only report the result:

$$H = \frac{1}{4} (2E_1 + 2E_2 + E_3 + E_4) + \frac{1}{4} (E_3 - E_4) (\sigma_{zI} - \sigma_{zO}) + \frac{1}{4} (2E_1 + 2E_2 - E_3 - E_4) \sigma_{zI} \sigma_{zO} \\ + \frac{1}{4} (E_1 - E_2) \left(\cos \frac{\alpha - \beta}{2} \right) (\sigma_{xI} \sigma_{xO} - \sigma_{yI} \sigma_{yO}) + \frac{1}{4} (E_1 - E_2) \left(\sin \frac{\alpha - \beta}{2} \right) (\sigma_{xI} \sigma_{yO} + \sigma_{yI} \sigma_{xO}). \quad (20)$$

The constant part of the Hamiltonian can be changed independently of the other coupling constants and it can be discarded. We can also generally vary the integers $N_{1,2,3,4}$ and the variables α , β , ρ , δ . The constant part is in fact proportional to $\mathcal{I}_I \otimes \mathcal{I}_O$. We avoid this notation and present the terms in the Hamiltonian in a more physically transparent form.

The Hamiltonian in (20) has also terms linear in the Pauli matrices (in the spin components for spin systems). These correspond to interactions with externally applied fields which in fact must be of opposite direction for the I

and O spins. As explained in the introduction, we try to avoid such interactions: hopefully, external fields will only be used for clocking of the computation, i.e., for controlling the internal interactions via some intermediary part of the system connecting the I and O two-state systems. Thus, we will assume that $E_3 = E_4$ so that there are no terms linear in the spin components.

Among the remaining interaction terms, the term involving the z -components in the product form $\sigma_{zI}\sigma_{zO}$ ($\equiv \sigma_{zI} \otimes \sigma_{zO}$), has an arbitrary coefficient to be denoted $-\mathcal{E}$. The terms of order two in the x and y components have free parameters similar to those in (11)-(12). The final expression is

$$H = -\mathcal{E}\sigma_{zI}\sigma_{zO} + \frac{\pi\hbar}{2\Delta t} \left(N - \frac{1}{2}\right) \left[(\cos\gamma) (\sigma_{xI}\sigma_{xO} - \sigma_{yI}\sigma_{yO}) + (\sin\gamma) (\sigma_{xI}\sigma_{yO} + \sigma_{yI}\sigma_{xO}) \right]. \quad (21)$$

Here $N = N_1 - N_2$ must be an integer. In order to minimize the spread of the energies E_1 and E_2 we could choose $|N - \frac{1}{2}| = \frac{1}{2}$. Recall that we already have $E_3 = E_4$. Thus the energy levels of the Hamiltonian in (21) are

$$E_1 = -\mathcal{E} + \frac{\pi\hbar}{\Delta t} \left(N - \frac{1}{2}\right), \quad E_2 = -\mathcal{E} - \frac{\pi\hbar}{\Delta t} \left(N - \frac{1}{2}\right), \quad E_{3,4} = \mathcal{E}. \quad (22)$$

Thus degeneracy of three levels (but not all four) can be achieved by varying the parameters.

The form of the interactions (21) is quite unusual as compared to the traditional spin-spin interactions in condensed matter models. The latter usually are based on the uniaxial (Ising) interaction proportional to $\sigma_z\sigma_z$, or the planar XY -model interaction proportional to $\sigma_x\sigma_x + \sigma_y\sigma_y$, or the isotropic (scalar-product) Heisenberg interaction. The spin components here are those of two different spins (not marked). The interaction (21) involves an unusually high degree of anisotropy in the system. The x and y components are coupled in a tensor form which presumably will have to be realized in a medium with well-defined directionality, possibly, a crystal.

5. COMMENT ON TIME-DEPENDENCE OF INTERACTIONS

The Hamiltonians considered thus far were all constant for the duration of the gate operation. We note that the external control of the interaction need not be limited to the time-dependence which is an abrupt on/off switching. Indeed, we can modify the time dependence according to

$$H(t) = f(t)H, \quad (23)$$

where we use the same symbol H for both the original time-independent interaction Hamiltonian such as (21) and the new, time-dependent one, $H(t)$. The latter involves the protocol function $f(t)$. The shape of this function, nonzero during the operation of the gate from time t to time $t + \Delta t$, can be smooth.

For Hamiltonians involving externally applied fields, such as (12), it may be important to have a constant plus an oscillatory components (corresponding to constant and electromagnetic-wave magnetic fields, for instance). However, the protocol function must satisfy

$$\int_t^{t+\Delta t} f(t') dt' = \Delta t, \quad (24)$$

and therefore it cannot be purely oscillatory; it must have a constant or other contribution to integrate to a nonzero value in accordance with (24).

The possibility of the modification (23) follows from the fact that the general relation

$$U = \left[e^{-i \int_t^{t+\Delta t} H(t') dt' / \hbar} \right]_{\text{time-ordered}} \quad (25)$$

does not actually require time ordering as long as the Hamiltonian commutes with itself at different times. This condition is satisfied by (23). Furthermore, if the Hamiltonian can be written as a sum of commuting terms then each term can be multiplied by its own protocol function. Interestingly, the Hamiltonian of the paramagnetic-resonance NOT gate¹⁴ is not of this form. It contains a constant part and an oscillatory part but they do not commute. Note that the term proportional to \mathcal{E} in (21) commutes with the rest of that Hamiltonian. The terms proportional to $\cos\gamma$ and $\sin\gamma$ do not commute with each other. Rather, they anticommute, in (21), as such terms do in (12).

6. THE THREE-SPIN XOR GATE

Thus far we learned that extending the number of spins (qubits, two-state systems) involved in the NOT gate from one to two produced an interaction Hamiltonian family (21) with structure that is quite new and unfortunately not symmetric in terms of what we are used to in solid-state magnetic interactions. We will now consider a *three-spin system*: a quantum-XOR gate (which can also be realized^{10,30,43} with two spins). This choice is dictated by the fact that we can obtain analytical results and address a new issue that was not there for one- or two-spin systems: whether this quantum gate function can be accomplished with two-spin interactions.

We note that if a quantum logic operation is allowed to be decomposed into a sequence of unlimited number of universal one- and two-spin gates then one can always reduce it to two-spin interactions.^{5,7,15,44} Here, however, we are interested in one-shot gates for which the external control involves the overall system Hamiltonian, over a single time interval Δt . The possibility of using solely two-spin interactions will actually depend on the logical function and for more complicated systems it has to be explored by numerical studies. We note also that the issue of having the interactions short-range (e.g., nearest-neighbor) does not really arise for few-spin systems although it will be an important design criterion as the number of spins (qubits) involved increases. Short-range two-particle interactions are much better studied and accessible to experimental probe than multi-particle interactions.

We denote by A, B, C the three two-state systems, i.e., three spins (qubits). The transformation must be specified for those initial states of the input spins A and B , at time t , that are one of the basis states $|AB\rangle = |11\rangle, |10\rangle, |01\rangle$, or $|00\rangle$, where 1 and 0 denote the eigenstates of the z -components of the spin operators. Here 1 refers to the up state and 0 refers to the down state; we use this notation for consistency with the classical bit notion. The initial state of C is not specified. We would like to have a quantum evolution that mimics the XOR function:

A	B	output
1	1	0
1	0	1
0	1	1
0	0	0

(26)

Here the output is at time $t + \Delta t$. One way to accomplish this is to produce the output in A or B , i.e., work with a two-spin system where the input and output are the same. The Hamiltonian for such a system is not unique. Explicit examples can be found^{10,30} where XOR was obtained as a sub-result of the controlled-NOT gate operation. In the case of two spins involved, the interactions can be single- and two-spin only.

Here we require that the XOR result be put in C at time $t + \Delta t$. The final states of A and B , as well as the phase of C are arbitrary. In fact, there are many different unitary transformations, U , that correspond to the desired evolution in the eight-state space with the basis $|ABC\rangle = |111\rangle, |110\rangle, |101\rangle, |100\rangle, |011\rangle, |010\rangle, |001\rangle, |000\rangle$. The choice of the transformation determines what happens when the initial state is a superposition of the reference states, what are the phases in the output, etc.

Let us consider first the following Hamiltonian^{31,32}

$$H = \frac{\pi\hbar}{4\Delta t} \left(\sqrt{2}\sigma_{zA}\sigma_{yB} + \sqrt{2}\sigma_{zB}\sigma_{yC} - \sigma_{yB}\sigma_{xC} \right). \quad (27)$$

It is written here in terms of the spin components; the subscripts A, B, C denote the spins. In the eight-state basis specified earlier, its matrix can be obtained by direct product of the Pauli matrices and unit 2×2 matrices \mathcal{I} . For instance, the first interaction term is proportional to $\sigma_{zA} \otimes \sigma_{yB} \otimes \mathcal{I}_C$. This Hamiltonian involves only two-spin-component interactions. In fact, in this particular example A and C only interact with B .

One can show that the Hamiltonian (27) corresponds to the XOR result in C at $t + \Delta t$ provided A and B were in one of the allowed superpositions of the appropriate binary states at t (we refer to superposition here because C is arbitrary at t). There are two ways to verify this.^{31,32} Firstly, one can diagonalize H and then calculate the evolution matrix U in the diagonal representation by using the general relation (7), valid for Hamiltonians which are constant during the time interval Δt , and then reverse the diagonalizing transformation.

The second, more general approach presented here is to design a whole family of two-spin-interaction Hamiltonians of which the form (27) is but a special case, by analyzing generally a family of 8×8 unitary matrices corresponding to the three-spin XOR gate. This program is carried out in Sections 7, 8.

7. THE STRUCTURE OF THE XOR UNITARY MATRIX AND HAMILTONIAN

We require any linear combination of the states $|\underline{111}\rangle$ and $|\underline{110}\rangle$ to evolve into a linear combination of $|\underline{110}\rangle$, $|\underline{100}\rangle$, $|\underline{010}\rangle$, and $|\underline{000}\rangle$; compare the underlined quantum numbers with the first entry in (26), with similar rules for the other three entries in (26). In the matrix notation, and in the standard basis $|ABC\rangle = |111\rangle, |110\rangle, |101\rangle, |100\rangle, |011\rangle, |010\rangle, |001\rangle, |000\rangle$, the most general XOR evolution operator corresponding to the Boolean function (26), with the output in C , is, therefore,

$$U = \begin{pmatrix} 0 & 0 & U_{13} & U_{14} & U_{15} & U_{16} & 0 & 0 \\ U_{21} & U_{22} & 0 & 0 & 0 & 0 & U_{27} & U_{28} \\ 0 & 0 & U_{33} & U_{34} & U_{35} & U_{36} & 0 & 0 \\ U_{41} & U_{42} & 0 & 0 & 0 & 0 & U_{47} & U_{48} \\ 0 & 0 & U_{53} & U_{54} & U_{55} & U_{56} & 0 & 0 \\ U_{61} & U_{62} & 0 & 0 & 0 & 0 & U_{67} & U_{68} \\ 0 & 0 & U_{73} & U_{74} & U_{75} & U_{76} & 0 & 0 \\ U_{81} & U_{82} & 0 & 0 & 0 & 0 & U_{87} & U_{88} \end{pmatrix}. \quad (28)$$

The condition of unitarity, $UU^\dagger = 1$, reduces the number of independent parameters but they are still too numerous for the problem to be manageable analytically; we are going to consider a subset of operators of this form.

From our earlier discussion we know that one way to reduce the number of parameters and ensure unitarity is to keep a single phase factor in each column and row of the matrix. Some amount of lucky guessing is involved in finding an analytically tractable parametrization. Thus, we choose a form which is diagonal in the states of the A -spin,

$$U = \begin{pmatrix} V_{4 \times 4} & 0_{4 \times 4} \\ 0_{4 \times 4} & W_{4 \times 4} \end{pmatrix}. \quad (29)$$

Note that the input spins A and B are not treated symmetrically. Here $0_{4 \times 4}$ denotes the 4×4 matrix of zeros. The 4×4 matrices V and W are parametrized as follows:

$$V = \begin{pmatrix} 0 & 0 & e^{i\delta} & 0 \\ e^{i\alpha} & 0 & 0 & 0 \\ 0 & 0 & 0 & e^{i\beta} \\ 0 & e^{i\gamma} & 0 & 0 \end{pmatrix}, \quad (30)$$

$$W = \begin{pmatrix} 0 & e^{i\rho} & 0 & 0 \\ 0 & 0 & 0 & e^{i\omega} \\ e^{i\xi} & 0 & 0 & 0 \\ 0 & 0 & e^{i\eta} & 0 \end{pmatrix}. \quad (31)$$

This choice of an 8-parameter unitary matrix U , see (29), was made because it has the structure

$$2U = (1 + \sigma_{zA})V + (1 - \sigma_{zA})W = V + W + \sigma_{zA}(V - W), \quad (32)$$

where V and W are operators in the space of B and C . Since U was chosen diagonal in the space of A , the Hamiltonian, H , will have a similar structure,

$$2H = P + Q + \sigma_{zA}(P - Q), \quad (33)$$

with the appropriate Hamiltonians P and Q in the $(B \otimes C)$ -space. In order to avoid three-spin interactions, $P - Q$ must be linear in the Pauli matrices. We also try to avoid single-spin (external-field) interactions. Thus, $P + Q$ must contain only terms of the second order in the spin components while $P - Q$ must contain only terms of the first order in the spin components. This suggests avoiding putting phase factors on the diagonal, which would lead to matrices similar to those encountered in extended-NOT-gate calculations that are known to be of a structure undesirable here: they contain a mixture of first-order and second-order terms. The off-diagonal choices remaining are considerably limited: the forms (30)-(31) are nearly unique.

In summary, while the arguments are admittedly vague and they do involve a certain level of guess, trial and error, the presented parametrization offers a good chance that with further restrictions on the parameters a two-spin interaction Hamiltonian can be obtained. As will be seen shortly, five conditions are imposed so that the resulting Hamiltonian depends on three (real) parameters.

Let us define

$$\mu = \frac{\alpha + \beta + \gamma + \delta}{4}, \quad \nu = \frac{\rho + \omega + \xi + \eta}{4}, \quad (34)$$

and introduce the reduced operators p and q ,

$$P = -\frac{\hbar}{\Delta t}p \quad \text{and} \quad Q = -\frac{\hbar}{\Delta t}q, \quad (35)$$

Then (7) yields

$$V = \exp(ip) \quad \text{and} \quad W = \exp(iq). \quad (36)$$

Next, we diagonalize V and W : we calculate their eigenvalues and also the matrices of their normalized eigenvectors, in order to transform to the diagonal representations.

Specifically, the eigenvalues of V are $e^{i\mu}$, $ie^{i\mu}$, $-e^{i\mu}$, $-ie^{i\mu}$. The appropriate eigenvalues of p then follow from (36) as μ , $\mu + \frac{1}{2}\pi$, $\mu + \pi$, $\mu + \frac{3}{2}\pi$. Arbitrary multiples of 2π can be added to these choices. However, there are certain nonrigorous arguments for generally keeping the spread of eigenvalues of the Hamiltonian as small as possible. Thus, we choose the simplest expressions. The eigenvalues of q are determined identically, with μ replaced by ν throughout.

The next step is to apply the inverse of the diagonalizing transformations for V and W to the diagonal 4×4 matrices for, respectively, p and q . The latter contain the eigenvalues of p and q as the diagonal elements. The results are the matrix forms of the operators p and q in the original representation:

$$\frac{4}{\pi}p = \begin{pmatrix} \frac{4}{\pi}\mu + 3 & -(1+i)e^{i(\mu-\alpha)} & -(1-i)e^{i(\delta-\mu)} & -e^{i(2\mu-\alpha-\gamma)} \\ -(1-i)e^{i(\alpha-\mu)} & \frac{4}{\pi}\mu + 3 & -e^{i(2\mu-\beta-\gamma)} & -(1+i)e^{i(\mu-\gamma)} \\ -(1+i)e^{i(\mu-\delta)} & -e^{i(\beta+\gamma-2\mu)} & \frac{4}{\pi}\mu + 3 & -(1-i)e^{i(\beta-\mu)} \\ -e^{i(\alpha+\gamma-2\mu)} & -(1-i)e^{i(\gamma-\mu)} & -(1+i)e^{i(\mu-\beta)} & \frac{4}{\pi}\mu + 3 \end{pmatrix}, \quad (37)$$

$$\frac{4}{\pi}q = \begin{pmatrix} \frac{4}{\pi}\nu + 3 & -(1-i)e^{i(\rho-\nu)} & -(1+i)e^{i(\nu-\xi)} & -e^{i(\rho+\omega-2\nu)} \\ -(1+i)e^{i(\nu-\rho)} & \frac{4}{\pi}\nu + 3 & -e^{i(\omega+\eta-2\nu)} & -(1-i)e^{i(\omega-\nu)} \\ -(1-i)e^{i(\xi-\nu)} & -e^{i(2\nu-\omega-\eta)} & \frac{4}{\pi}\nu + 3 & -(1+i)e^{i(\nu-\eta)} \\ -e^{i(2\nu-\rho-\omega)} & -(1+i)e^{i(\nu-\omega)} & -(1-i)e^{i(\eta-\nu)} & \frac{4}{\pi}\nu + 3 \end{pmatrix}. \quad (38)$$

8. THE TWO-SPIN-INTERACTION XOR HAMILTONIAN

Thus far we decreased the number of independent parameters in the general unitary transformation and chose it to be diagonal in the A -space. We now refine our design of the Hamiltonian to favor interaction of the second order in the Pauli matrices. First, we note that both P and Q are constant-diagonal matrices. Therefore, in terms of the Pauli matrices both their sum and difference in (33) will involve constant terms. These are undesirable because in $\sigma_{zA}(P-Q)$ they lead to terms of order one (instead of the desired two), in H , while in $P+Q$ they lead to an additive constant in H which only affects the overall phase of the unitary transformation and is of no interest otherwise. Therefore, we put

$$\mu = \nu = -\frac{3}{4}\pi, \quad (39)$$

in order to nullify these diagonal elements in both P and Q .

Let us now focus our attention on $P-Q$ which, by (39), is now a matrix with zero diagonal. We must impose conditions on the parameters to make $P-Q$ of order exactly one in the Pauli matrices. We note, however, that due to zero-diagonal, it cannot contain σ_z terms. The general form linear in σ_x, σ_y is

$$P-Q = \mathcal{I}_B \otimes \begin{pmatrix} 0 & X \\ X^* & 0 \end{pmatrix}_C + \begin{pmatrix} 0 & Y \\ Y^* & 0 \end{pmatrix}_B \otimes \mathcal{I}_C = \begin{pmatrix} 0 & X & Y & 0 \\ X^* & 0 & 0 & Y \\ Y^* & 0 & 0 & X \\ 0 & Y^* & X^* & 0 \end{pmatrix}, \quad (40)$$

where the stars denote complex conjugation, X and Y are arbitrary (complex) numbers, and \mathcal{I} stands for the unit matrix as before. Thus we require that $P-Q$ be of the form suggested by (40). This imposes several conditions: two above-diagonal elements of the difference must be equal to zero while the remaining four elements must be equal pairwise. One can show that these conditions are satisfied provided α, β, γ are kept as three independent (real) parameters while the remaining angles are given by

$$\delta = -3\pi - \alpha - \beta - \gamma, \quad (41)$$

$$\rho = -\pi + \beta, \quad (42)$$

$$\omega = -2\pi - \alpha - \beta - \gamma, \quad (43)$$

$$\xi = -\pi + \gamma, \quad (44)$$

$$\eta = \pi + \alpha. \quad (45)$$

Note that (39) is built into (41)-(45). Given this choice, it turns out that $P+Q$ contains only two-spin interactions. We have no simple explanation of this property (of the absence of first-order terms in $P+Q$). It is probably related to the fact that the structure pattern of the original matrices V and W is quite similar even though the precise positioning of nonzero elements is different. We find

$$P+Q = -\frac{\sqrt{2}\pi\hbar i}{4\Delta t} \begin{pmatrix} 0 & e^{-i\alpha} + e^{i\beta} & e^{-i(\alpha+\beta+\gamma)} - e^{-i\gamma} & -\sqrt{2}e^{-i(\alpha+\gamma)} \\ -e^{i\alpha} - e^{-i\beta} & 0 & -\sqrt{2}e^{-i(\beta+\gamma)} & e^{-i\gamma} - e^{-i(\alpha+\beta+\gamma)} \\ e^{i\gamma} - e^{i(\alpha+\beta+\gamma)} & \sqrt{2}e^{i(\beta+\gamma)} & 0 & -e^{-i\alpha} - e^{i\beta} \\ \sqrt{2}e^{i(\alpha+\gamma)} & e^{i(\alpha+\beta+\gamma)} - e^{i\gamma} & e^{i\alpha} + e^{-i\beta} & 0 \end{pmatrix}, \quad (46)$$

$$P-Q = -\frac{\sqrt{2}\pi\hbar i}{4\Delta t} \begin{pmatrix} 0 & e^{-i\alpha} - e^{i\beta} & e^{-i(\alpha+\beta+\gamma)} + e^{-i\gamma} & 0 \\ -e^{i\alpha} + e^{-i\beta} & 0 & 0 & e^{-i(\alpha+\beta+\gamma)} + e^{-i\gamma} \\ -e^{i(\alpha+\beta+\gamma)} - e^{i\gamma} & 0 & 0 & e^{-i\alpha} - e^{i\beta} \\ 0 & -e^{i(\alpha+\beta+\gamma)} - e^{i\gamma} & -e^{i\alpha} + e^{-i\beta} & 0 \end{pmatrix}, \quad (47)$$

Finally, we expand these matrices in terms of products of the Pauli matrices and collect terms according to (33) to get

$$\begin{aligned}
H = -\frac{\pi\hbar}{8\Delta t} \Big\{ & \sqrt{2}(\sin\alpha + \sin\beta)\sigma_{zA}\sigma_{xC} - \sqrt{2}(\cos\alpha - \cos\beta)\sigma_{zA}\sigma_{yC} + \sqrt{2}[\sin\gamma + \sin(\alpha + \beta + \gamma)]\sigma_{zA}\sigma_{xB} \\
& - \sqrt{2}[\cos\gamma + \cos(\alpha + \beta + \gamma)]\sigma_{zA}\sigma_{yB} + \sqrt{2}(\sin\alpha - \sin\beta)\sigma_{zB}\sigma_{xC} - \sqrt{2}(\cos\alpha + \cos\beta)\sigma_{zB}\sigma_{yC} \\
& - \sqrt{2}[\sin\gamma - \sin(\alpha + \beta + \gamma)]\sigma_{xB}\sigma_{zC} + \sqrt{2}[\cos\gamma - \cos(\alpha + \beta + \gamma)]\sigma_{yB}\sigma_{zC} - [\sin(\alpha + \gamma) + \sin(\beta + \gamma)]\sigma_{xB}\sigma_{xC} \\
& + [\cos(\alpha + \gamma) - \cos(\beta + \gamma)]\sigma_{xB}\sigma_{yC} + [\cos(\alpha + \gamma) + \cos(\beta + \gamma)]\sigma_{yB}\sigma_{xC} + [\sin(\alpha + \gamma) - \sin(\beta + \gamma)]\sigma_{yB}\sigma_{yC} \Big\}. \quad (48)
\end{aligned}$$

Note that (27) corresponds to the parameter choice $\alpha = \beta = \gamma = 0$. The Hamiltonian (48) describes the three-spin XOR. For arbitrary values of α, β, γ , the interactions involved are all two-spin as desired. The result, however, is not symmetric in any obvious way. It seems to correspond to complicated tensor interactions involving expressions of order two in the components of the three spins involved. No rotational or other symmetry in the three-component spin space, or planar symmetry, or uniaxial coupling, are apparent. All these would correspond to the familiar Heisenberg, XY , and Ising couplings in condensed matter physics.

Thus, in order to realize interaction (48) in materials, a rather anisotropic medium with highly nonsymmetric tensorial magnetic interactions will be required. In this respect our analytical attempt to design a multi-spin quantum gate cannot be considered really successful. While we learned several general principles, the unappealing form of the Hamiltonians (21) and (48) suggests that different roots to the derivation of Hamiltonians should be also explored. One could start with the more conventional magnetic interactions, isotropic (Heisenberg), planar (XY), uniaxial (Ising), and explore general-parameter Hamiltonians, adjusting the coupling parameters numerically in search of those values for which useful Boolean gate operations are carried out. Another approach would be to use, in input and output, quantum states more general than the logic products of the qubit-basis-states which are presently favored because of the correspondence with classical computers. Then the design of Hamiltonians may be easier but there is a trade-off. These devices will have to be incorporated into larger computers or interact with classical (i.e., dissipative) computer components. Radically new programming ideas will be needed to use transformations that connect *superpositions* of qubit states to carry out computations.

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